

Modeling coupled biogeochemical cycles

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Organisms require about 30 essential elements to sustain life. The cycles of these elements are coupled to one another through the specific physiological requirements of the organisms. Here, I contrast several approaches to modeling coupled biogeochemical cycles using an example of carbon, nitrogen, and phosphorus accumulation in a Douglas-fir (*Pseudotsuga menziesii*) forest ecosystem and the response of that forest to elevated atmospheric carbon dioxide concentrations and global warming. Which of these approaches is most appropriate is subject to debate and probably depends on context; nevertheless, this question must be answered if scientists are to understand ecosystems and how they might respond to a changing global environment.

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To ensure normal growth and maintain routine life processes, organisms must continually obtain about 30 essential elements from their environment (eg carbon [C], nitrogen [N], phosphorus [P]). Furthermore, organisms require these elements in fairly constrained relative proportions (Sterner and Elser 2002). Largely through the actions of organisms, these essential elements are continuously recycled and – because of the constrained proportions required for life – element cycles are inextricably coupled to one another. The approaches to modeling this coupling are, however, as varied as the scientists developing the models. In this paper, I examine three ways to represent coupled biogeochemical cycles in dynamic simulation models and demonstrate the consequences of those choices.

Modeled biogeochemical cycles are often linked to one another through the equations used to describe the growth of the component organisms. A classic way to represent this linkage is to assume that growth is constrained only by the most limiting of the resources needed for growth (Liebig's Law of the Minimum; eg Tilman 1977; Loladze *et al.* 2000; Grover 2004; Haefner 2005). With a Liebig formulation, control of the linkages among cycles switches from one resource to another as the different resources in turn become limiting to growth.

An alternative way to represent these linkages is to model organism growth as being limited by several

resources at the same time. There are many ways to represent this “concurrent limitation” (see O'Neill *et al.* 1989; Haefner 2005). The archetype for this diverse class of models is one in which growth is proportional to the *product* of several factors representing the availability of various resources in the environment (eg Droop 1973; Diehl *et al.* 2005). With this concurrent formulation, control of the linkages among resource cycles is shared among resources, and the capacity for uptake of one resource increases as the availability of any of the other resources increases.

A third way to model these linkages is an “acclimating formulation”, in which the model organisms adjust their capacity to acquire various resources, optimizing the relative proportions of the resources taken up (eg Thornley 1972; Vallino *et al.* 1996; Rastetter *et al.* 1997; Kooijman 2001). As with those related to the concurrent formulation, the strengths of the linkages in the acclimating formulation vary as resource concentrations change, but with a lag associated with the time needed to acclimate to the changes in resource concentrations. The adjustment of acquisition capacity evolves to increase uptake of the most limiting resource and to decrease uptake of the less limiting resources, resulting in long-term dynamics that resemble a Liebig-like response (Rastetter and Shaver 1992).

■ Model description

To illustrate these approaches to coupling biogeochemical cycles, I built a simple model of the C, N, and P cycles in a Douglas-fir (*Pseudotsuga menziesii*) forest and parameterized it to data reported by Sollins *et al.* (1980), with the assumption that the forest they described was at a steady state (Figure 1; see WebPanel 1 for further details about model equations, parameters/variables, etc). The model had C, N, and P stocks for plants (B_C , B_N , and B_P), leaf litter, soil organic matter (SOM), and associated microbes (D_C , D_N , and D_P), as well as stocks of inorganic N and P (E_N and E_P). Carbon entered the ecosystem only through net primary production (NPP;

In a nutshell:

- The cycles of elements essential to life on Earth are inextricably linked to one another
- There are several ways of modeling how biogeochemical cycles are coupled
- Different approaches to modeling coupled element cycles result in very different predictions of ecosystem function
- The most suitable approach to modeling coupled element cycles remains an open question, and the answer is most likely context dependent

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P_n), was transferred to soils through litter fall (L_C), and was lost from the ecosystem through microbial respiration (R_m) and dissolved organic matter loss (Q_{OC}). Nitrogen entered the ecosystem both through deposition to the inorganic pool (I_{ND}) and through both symbiotic and non-symbiotic N fixation (U_{Nfix} and I_{NF}). Inorganic N was taken up by plants (U_N) and cycled back to the soil via litter fall (L_N). In the soil, microbes exchanged N between organic and inorganic stocks through mineralization (M_N) and immobilization (U_{mN}); N was lost from the ecosystem in both inorganic (Q_N) and organic (Q_{ON}) forms. The P cycle was identical to that of N, except that there was no analog to N fixation. An important feature of both the N and P cycles in this and many other ecosystems is that well over 90% of the N and P requirements for vegetation is supplied from sources recycled within the ecosystem.

As plant biomass accumulates, the relative abundance of different tissues in the forest changes so that active tissues (B_A) such as leaves and roots transition from constituting a major component of the biomass in a very young forest to comprising only a very small component as woody tissues (B_W) come to dominate at maturity. I accounted for these changes with a simple allometric equation (see WebPanel 1). I assumed element uptake rates increase in proportion to active biomass and a Michaelis–Menten function of element concentration. Also, because woody tissues have much higher C:N and C:P ratios (810 g C g⁻¹ N and 6250 g C g⁻¹ P; Sollins *et al.* 1980) than those in active tissues (59 g C g⁻¹ N and 286 g C g⁻¹ P), I included equations to increase the optimal C:N and C:P ratios to reflect the changes in allometry. I also assumed that the optimal element proportions of soil microbes – and hence microbial C, N, and P requirements – remained constant (8 g C per gram of N [Brady 1974]; 56 g C per gram of P, assumes a 16:1 molar ratio). However, I did allow for variation in the C:N:P ratios of the SOM.

The model consisted of simple 1st-order differential equations representing the mass balance for the C, N, and P stocks. I integrated these equations with an adaptive-time-step, 4th- and 5th-order Runge–Kutta numerical integrator, with the time-step adaptation set to ensure an accuracy of better than 0.01% (Press *et al.* 1986).

The model could be run in four configurations that differed in resource uptake by plants (P_n , U_N , and U_P) and microbes (U_{mN} and U_{mP}). Secondary couplings included: mineralization and microbial respiration, which were calculated from U_{mN} and U_{mP} to maintain microbial element ratios; symbiotic N fixation, which was activated if N was more limiting to plants than either C or P and the canopy was open enough to support N-fixing plants; and non-symbiotic N fixation, which increased in proportion to wood surface area to reflect increases in surfaces for N-fixing lichens and the availability of a high C:N ratio in litter for N-fixing bacteria. The four configurations were as follows (see also WebPanel 1):

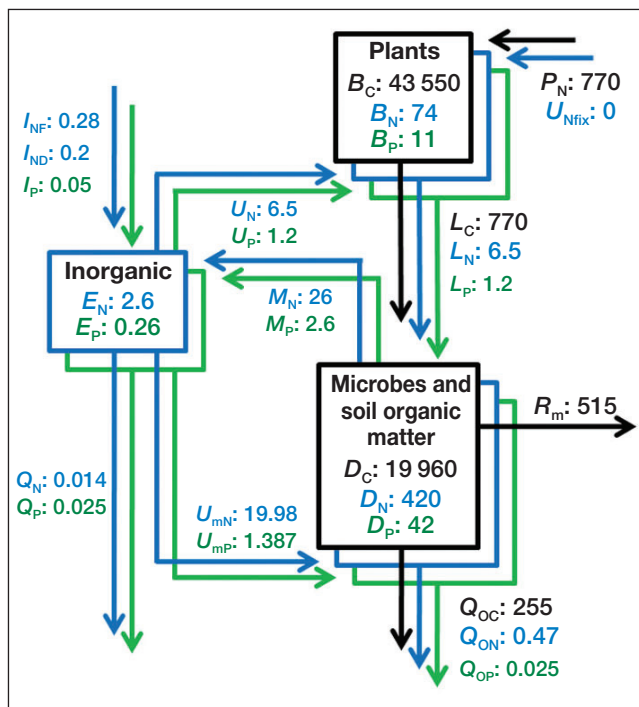


Figure 1. A simple model of C, N, and P cycling in a mature Douglas-fir forest. Fluxes are defined in the text. All stocks are in g m⁻² and all fluxes in g m⁻² yr⁻¹.

- (1) *Uncoupled*: I simulated the C cycle as being independent of the N and P cycles.
- (2) *Liebig*: I calculated uptake rates for C, N, and P as if the cycles were uncoupled, to determine which of the three resources was most limiting. I then set the growth rates for plants and microbes to their respective most-limited rates, and calculated the uptake rates of the other two resources to maintain the optimal element ratios.
- (3) *Concurrent limitation*: I calculated NPP as proportional to the product of the uncoupled uptake rates, using the equation:

$$P_n^* = \rho_M P_n (U_N + U_{Nfix}) U_P / B_A^2 \quad (\text{Eq 1}),$$

where $*$ indicates the NPP for the concurrent configuration, ρ_M is a weighting constant, and the division by B_A^2 is to correct for the triple accounting of active biomass on uptake. I then calculated N and P uptake and N-fixation rates to maintain the optimal plant element ratios. For microbes, I calculated C uptake proportional to the product of the C uptake rate, the inorganic plus organic N uptake rate, and the inorganic plus organic P uptake rate. As with the plants, I calculated N and P uptake rates to maintain the optimal microbial element ratios.

(4) *Acclimating*: I calculated plant uptake rates as the uncoupled rates multiplied by a factor (V_i), representing the fraction of uptake assets allocated to the uptake of each resource. These assets include biomass, enzymes, and carbohydrates that the plant can allocate toward the acquisition of resources from the environment. The V_i acclimated based on the uptake (U_i) relative to requirement for that

element (R_i). This requirement is the amount of the element lost in litter multiplied by a factor to correct for deviations of the element ratios in the biomass from an optimum. The allocation equation I used was:

$$dV_i/dt = a \ln(\Psi R_i/U_i) V_i \quad (\text{Eq 2}),$$

where a is an acclimation rate constant and Ψ is calculated to ensure that the sum of the dV_i/dt equals zero and hence the sum of the V_i equals one:

$$\Psi = \prod_{i=1}^3 (U_i/R_i)^{V_i} \quad (\text{Eq 3}).$$

The acclimations equation (Eq 2) simply redistributes uptake assets away from non-limiting resources ($\Psi R_i < U_i$) and toward limiting ones ($\Psi R_i > U_i$). The logarithmic formulation scales acclimation to deviations in element ratios rather than to absolute differences (see Rastetter and Shaver 1992). I used a similar approach for microbes, except that I assumed acclimation was infinitely fast and therefore set the distribution of uptake assets to the optimal distribution at all times. In addition to the time lag associated with acclimation, the acclimating and concurrent-limitation models differ fundamentally in their response to element availability. For example, if the three elements are at their respective half-saturation concentrations and those concentrations are increased to saturating levels, the uptake rates in the concurrent-limitation

model will all increase by a factor of eight, which represents a doubling for each of the three elements. Alternatively, with the acclimating configuration, the rates will only double and, because the relative uptakes will remain in balance, there will be no subsequent acclimation to change those rates.

I calibrated all four configurations to data in Sollins *et al.* (1980; Figure 1; WebPanel 1) and ran three sets of simulations. First, I modeled primary succession by cutting the initial plant biomass and SOM to 1% of their steady-state values and allowing the ecosystem to recover over 2000 years (Figure 2). I set initial P inputs to $0.4 \text{ g P m}^{-2} \text{ yr}^{-1}$ and decreased them linearly to $0.2 \text{ g P m}^{-2} \text{ yr}^{-1}$ by year 200 and to the $0.05 \text{ g P m}^{-2} \text{ yr}^{-1}$ value reported by Sollins *et al.* (1980) by year 1000. Without an analog of N fixation, it is impossible to accumulate biomass and soils at the observed rate without imposing this increased P input to the ecosystem early in succession.

Model output

The four simulations differed substantially in the rates of C, N, and P accumulation in plants and soils during primary succession (Figure 2). Without nutrient limitation, plant C in the uncoupled model accumulated to the steady-state levels within a few hundred years and soil C within 1000 years; this was faster than the rates reported by Bormann and Sidle (1990) for Glacier Bay, Alaska.

This accumulation rate is limited only by photosynthetic capacity, which itself increases as plant biomass increases. Accumulation is slower in soil than in vegetation because C has to pass through vegetation before entering the soil.

With the Liebig configuration, plant biomass and SOM accumulated more slowly than in any other configurations or the Bormann and Sidle (1990) data (Figure 2). This accumulation rate was limited by N, except between years 80–140, when symbiotic N fixation helped to fulfill the N requirements of the plants. During this N-fixing phase, NPP limited the maximum rate of symbiotic N fixation and, consequently, limited the accumulation rate of biomass and SOM. Nitrogen fixation peaked at $1.8 \text{ g N m}^{-2} \text{ yr}^{-1}$ and cumulatively contributed about 10% of the N entering the ecosystem. After year 140, the accumulation rate of biomass and SOM in the Liebig configuration decreased sharply. This rate was determined by the rate of N deposition and non-symbiotic N fixation minus the accelerating rates of organic and inorganic N losses as the N stocks accumulate; P was never limiting.

In the concurrent-limitation simulation, the multiplicative effect of the three resources

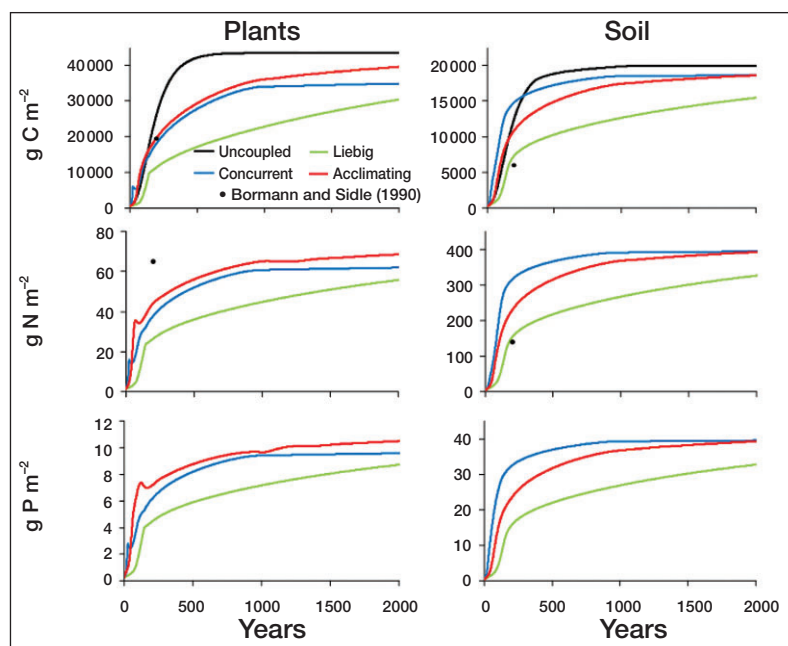


Figure 2. Accumulation of C, N, and P in plants and soils during primary succession, as predicted by four models. The uncoupled model assumes the C cycle is independent of the nutrient cycles. The Liebig model assumes plant and microbial growth are constrained only by the most limiting resource. The concurrent-limitation model assumes plant and microbial growth increase in proportion to the product of the availabilities of all resources (eg Eq 1). The acclimating model redistributes uptake assets among resources to optimize growth. The Bormann and Sidle (1990) data are for a 200-year-old site in Glacier Bay, Alaska.

on uptake allowed the plants to increase the N uptake capacity, which effectively depleted inorganic N stocks during the first 85 years of the simulation. The deficit was made up by symbiotic N fixation, which initiated within the first 2 years of the simulation and thus much earlier than predicted with the Liebig configuration. Nitrogen fixation rate increased to a sharp peak at $2.9 \text{ g N m}^{-2} \text{ yr}^{-1}$ in year 21, declined by 50% over the next 6 years, and then increased to another peak of $2.8 \text{ g N m}^{-2} \text{ yr}^{-1}$ in year 85. Between these two peaks, inorganic P concentration fell below 0.26 g P m^{-2} , the concentration used for the steady-state calibration. Cumulatively, symbiotic N fixation contributed 30% of the N entering the ecosystem. With concurrent limitation, it is difficult to identify a single factor restricting biomass accumulation; however, inorganic N never increased above 50% of the concentration in the steady-state calibration, whereas after year 85, P remained above its calibration concentration. Nevertheless, the role of P in limitation can be seen in the sharp decline in biomass accumulation at year 1000, the year that supplemental P input to the system ceased. These patterns suggest that although N is the ultimate limiting factor, elevated P increases the N uptake capacity and thereby partially eases the N limitation. Early nutrient limitation is also obvious in the fast SOM accumulation; the low nutrient availability slowed microbial activity and thereby slowed C loss via respiration. Also, with concurrent limitation, inorganic nutrients stimulate the release of nutrients from organic matter. Thus, nutrient limitation favors fast N and P accumulation in SOM.

With the acclimating configuration, neither inorganic N nor P was depleted as much during early succession as each was in the concurrent-limitation model. Yet symbiotic N fixation was initiated within the first few years of the simulation and increased steadily, to a peak of $2.8 \text{ g N m}^{-2} \text{ yr}^{-1}$ in year 56. Cumulatively, symbiotic N fixation contributed 12% of the N entering the ecosystem. In the model, acclimation redistributes uptake assets until the ratio of uptake to requirement is the same for all resources. In that sense, all resources are equally limiting. Because of this optimization, biomass accumulated slightly faster here than in the concurrent-limitation simulation, and the rate of accumulation decreased less at year 1000, when supplemental P inputs ceased. The effect of the optimized resource acquisition is also obvious in the SOM accumulation, which proceeded more slowly despite higher inputs from vegetation through higher microbial activity.

■ Simulation results for elevated CO_2 and warming

I ran two more sets of 100-year simulations, in which I (1) doubled CO_2 and (2) doubled CO_2 and warmed the ecosystem by 4°C . I assumed that plant and microbial N and P uptake and microbial use of organic C, N, and P increased 32% with the 4°C warming ($Q_{10} = 2$, where

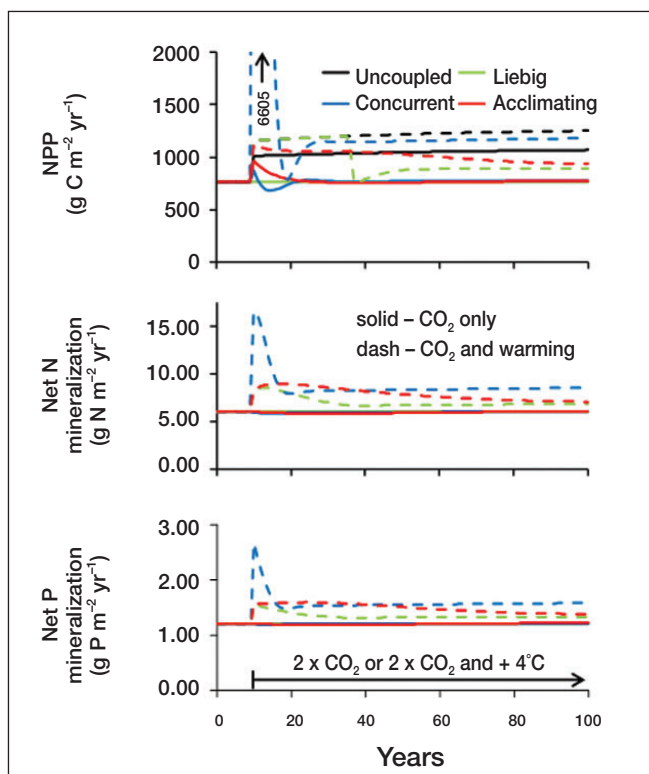


Figure 3. Changes in element flux rates in response to a doubling of atmospheric CO_2 (solid lines) and to a doubling of CO_2 and a 4°C warming (dashed lines) as predicted by four biogeochemical models. Models are as defined in Figure 2.

Q_{10} is the factor by which the metabolic rate increases with each 10°C increase in temperature) and that NPP increased 14% ($Q_{10} = 1.4$). Both sets of simulations began with the forest at the calibrated steady state (Figures 3 and 4).

Doubling CO_2 alone caused an instantaneous increase in NPP of about 30% in all but the Liebig configuration (Figure 3), where nutrient limitation did not allow that model to respond to elevated CO_2 alone. In the uncoupled configuration, the elevated NPP increased slightly with time as more photosynthetic biomass was added to the vegetation. When CO_2 increased, the N and P uptake capacity increased instantaneously in the concurrent configuration and increased within a few years in the acclimating configuration. However, no matter how much this uptake capacity increases, uptake itself cannot be maintained in the long term above the rate of supply. Thus, nutrient limitation maintained by the relatively constant rates of net N and P mineralization caused N and P uptake, and therefore NPP, to drop back down to near their initial rates in the concurrent and acclimating configurations; after 100 years, NPP was less than 1% above the initial values. Contrary to this rapid down-regulation of NPP, NPP at Duke University's free-air CO_2 enrichment (FACE) experiment remained about 20% above ambient for at least 8 years (McCarthy *et al.* 2010); however, the Duke FACE site is much younger and more fertile than the Douglas-fir site used here. Elevating CO_2

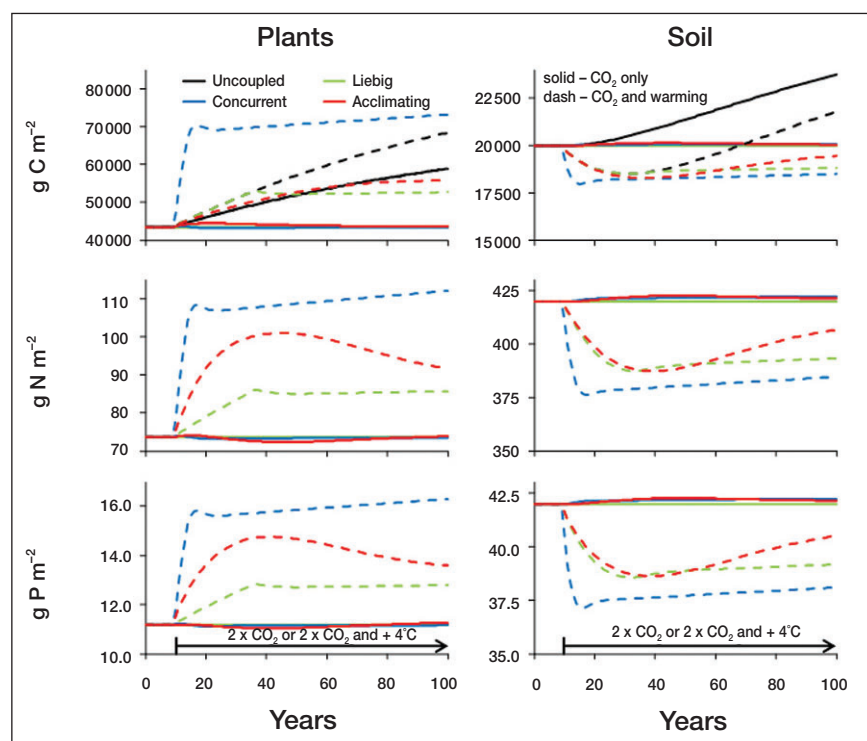


Figure 4. Changes in ecosystem C, N, and P stocks in response to a doubling of atmospheric CO₂ and to a doubling of CO₂ and a 4°C warming as predicted by four biogeochemical models. Models are as defined in Figure 2.

concentrations resulted in substantial increases in plant and soil C stocks only in the uncoupled configuration, where the C cycle was not constrained by nutrient limitation (Figure 4).

In the uncoupled model, direct stimulation of NPP is about 50% greater with both CO₂ and warming than with CO₂ alone, resulting in commensurate increases in plant biomass (Figures 3 and 4). Warming does cause an initial loss of soil C, but that C is recovered within about 60 years, after which soils become a net sink for C. For the remaining models, warming in conjunction with elevated CO₂ levels resulted in much stronger responses than elevated CO₂ levels alone, because warming increases the rate of nutrient cycling. The effect of elevated CO₂ and warming on net nutrient mineralization involves several factors acting in concert, including the direct effects of warming on metabolism and the secondary effects elicited by elevated CO₂ on plant nutrient demand and plant nutrient uptake. As a result, the net nutrient mineralization can be substantially higher than the 32% increase expected from warming alone (Figure 3). The increase in nutrient availability allowed all of these models to increase NPP more than with elevated CO₂ alone – especially in the concurrent-limitation model, where the direct effects of CO₂ and warming on NPP, the effects of warming on nutrient uptake potential, and the increase in nutrient availability resulted in a 750% increase in NPP. There was a subsequent down-regulation of NPP in all of these models. Unlike the succession simulations, where N was the dominant limiting factor, the down-regulation of NPP was driven by a depletion of P. The reason that

P, rather than N, drives this response is that the plant response is sustained by soil-derived nutrients; in the Sollins *et al.* (1980) data, there is about 50% more N than P in soils relative to plant requirements (ie soil N:P is 50% higher than plant N:P). In all of these simulations, the responses to elevated CO₂ and warming resulted in an increase in plant biomass and in total ecosystem C (Figure 4). This increase in total ecosystem C was largely possible because of a net redistribution of nutrients from soils (with low C-to-nutrient ratios) to plants (with high C-to-nutrient ratios). The responses also resulted in a net 1% increase in ecosystem N and a net 2% increase in ecosystem P in the concurrent-limitation and acclimating models; in the Liebig model, the ecosystem lost about 3% of its N and 2% of its P.

Conclusions

The mode of coupling biogeochemical cycles clearly has a substantial effect on the simulated biogeochem-

istry of ecosystems, and these effects are manifested very differently depending on the context (eg succession versus response to elevated CO₂ concentrations and warming). However, which model best describes real ecosystems remains an open question – one that is difficult to answer because of the long response times of ecosystems. Indeed, the solution might depend on context; a Liebig formulation, for example, might be a perfectly adequate description in an agronomical context but would be inappropriate in a global-change context. The question will nevertheless need to be answered if scientists are to understand the mechanisms underlying ecosystem behavior and be able to make reliable projections of how ecosystems will respond to long-term changes in atmospheric chemistry, climate, and land use.

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